Example 1a

June 17, 2020

1 Example 1a: Harmonic trap - Training of DeepCalib

Example code to train DeepCalib to determine the stiffness of a Brownian particle system in a harmonic trap.

DeepCalib 1.0 Enhanced force-field calibration via machine learning version 1.0 - 27 April 2020 l' Aykut Argun, Tobias Thalheim, Stefano Bo, Frank Cichos & Giovanni Volpe Soft Matter Lab

1.1 1. INIZIALIZATION

```
In [1]: import DeepCalib
```

1.2 2. DEFINE TRAJECTORY SIMULATION

Here the function that simulates the motion of the Brownian particle in the force field under consideration is defined. Specifically, in this case, we consider a Brownian particle in a harmonic force field, and the motion of the particle depends on the trap stiffness k.

This file is used to reproduce results that are shown in Fig.1 and generate the pretrained network "DeepCalib_Example 1a.h5" that is going to be needed to execute Example 1b.

Comments: 1. The function that simulates the trajectories must be called simulate_trajectory. 2. Lambda functions scale_inputs, rescale_inputs, scale_targets, and rescale_targets must also be defined. For the best performance of the learning, the rescaling of both the inputs and targets should lead to values of order 1.

```
In [2]: ### Physical parameters
        from math import pi
        R = 1e-7
                                   # Radius of the Brownian particle [m]
                                   # Viscosity of the medium [kg m^-1 s^-1]
        eta = 0.001
        T = 300
                                   # Temperature [K]
        k0 = 10
                                   # Reference stiffness [fN \mu m ^-1]
        gamma0 = 6 * pi * eta * R # Reference friction coefficient [kq s^-1]
        ### Simulation parameters
        N = 1000
                                   # Number of samples of the trajectory
        Dt = 1e-2
                                   # Timestep
        oversampling = 5
                                 # Simulation oversampling
                                   # Number of equilibration timesteps
        offset = 1000
```

```
### Define functions to scale and rescale inputs
                                                     # Scales input trajectory to order
scale_inputs = lambda x: x * 1e+6
rescale_inputs = lambda scaled_x: scaled_x * 1e-6
                                                    # Rescales input trajectory to phys
### Define function to scale and rescale targets
from numpy import log
from numpy import exp
scale_targets = lambda k: log(k / k0)
                                                                     # Scales targets to
rescale_targets = lambda scaled_k: exp(scaled_k) * k0
                                                                     # Inverse of targets
### Define the simulate_trajectory function
def simulate_trajectory(batch_size=32,
                        T=T,
                        k0=k0,
                        gamma0=gamma0,
                        N=N.
                        Dt=Dt,
                        oversampling=oversampling,
                        offset=offset,
                        scale_inputs=scale_inputs,
                        scale_targets=scale_targets):
    """Simulates a Brownian particle in a harmonic trap
    Inputs:
    T:
                    temperature of the environment
    k0:
                    center of the stiffness range
                    friction coefficient
    gamma0:
    N:
                    number of trajectory data points
    Dt:
                    measurement period
    oversampling:
                    oversampling from the simulation time step (to calculate dt)
                    steps of the simulation before starting to save the trajectory
    offset:
                    inputs scale function for the network, to normalize it comparable to
    scale_inputs:
    scale_targets: targets scale function for the network, to normalize it comparable t
    Outputs:
    inputs: the inputs for the network, these are trajectories that have the following j
            inputs.names:
                                   names of the input trajectory variables ('x', 'y' etc
```

targets: the expected ground truth measurements for the trajectory that have follows

values of the inputs in SI units

inputs.scaled_values: scaled values of the inputs to be passed to the netwo

short description of the scaling function for the inp

inputs.values:

inputs.scalings:

```
names of the targets to be measures ('k' etc)
        targets.names:
        targets.values:
                              values of the ground truth targets in SI units
        targets.scalings:
                              short description of the scaling function for the to
        targets.scaled_values: scaled values of the ground truth targets to be pass
11 11 11
import numpy as np
from scipy.constants import Boltzmann as kB
from math import pi
from math import sqrt
from numpy.random import randn as gauss
from numpy.random import rand as uniform
### Randomize trajectory parameters
k = k0 * (10**(uniform(batch_size) * 3 - 1.5)) # Generates random stiffness value
gamma = gamma0 * (uniform(batch_size) * .1 + .95) # Marginal randomization of frict
### Simulate
                                       # time step of the simulation
dt = Dt / oversampling
x = np.zeros((batch_size, N))
                                       # initialization of the x array
D = kB * T / gamma
                                       # diffusion coefficient
C1 = -k *1e-9 / gamma * dt
                                             # drift coefficient of the Langevin equ
C3 = np.sqrt(2 * D * dt)
                                     # random walk coefficient of the Langevin equ
X = x[:, 0]
n = 0
                                             # Offset (for some prerun before running
for t in range(offset):
    X = X + C1 * X + C3 * gauss(batch_size)
for t in range(N * oversampling):
                                             # Simulation
    X = X + C1 * X + C3 * gauss(batch_size)
    if t % oversampling == 0:
                                             # We save every oversampling^th values
        x[:, n] = X
        n += 1
# Normalize trajectory and targets
inputs = DeepCalib.trajectory(
    names=['x'],
    values=x,
    scalings=['x [\u03BCm]'],
    scaled_values=scale_inputs(x))
targets = DeepCalib.targets(
    names=['k [fN/\u03BCm]'],
    values=k,
```

```
scalings=['log(k / k0)'],
scaled_values=scale_targets(k))
```

return inputs, targets

1.3 3. CHECK TRAJECTORY SIMULATION

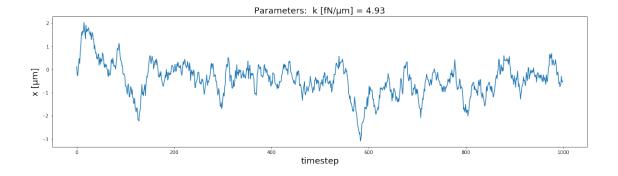
Checks the results of the function to simulate the trajectories by plotting some examples in rescaled units.

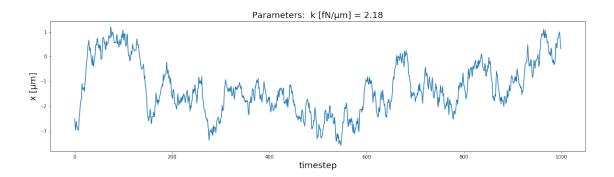
Have a look at the trajectories and check if they match your system, and keep an eye on different trajectories and make sure your scaled units vary in the order of 1, i.e, neither too small (0.01 or smaller) nor too large (100 or larger)

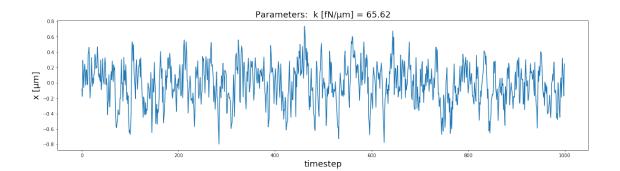
The parameter number_of_images_to_show determines the number of trajectories that are plotted.

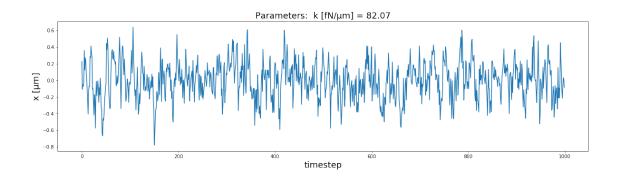
In [3]: ### Show some examples of simulated trajectories

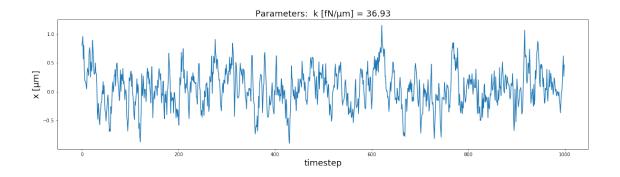
```
number_of_trajectories_to_show = 10
%matplotlib inline
DeepCalib.plot_sample_trajectories(simulate_trajectory, number_of_trajectories_to_show)
```

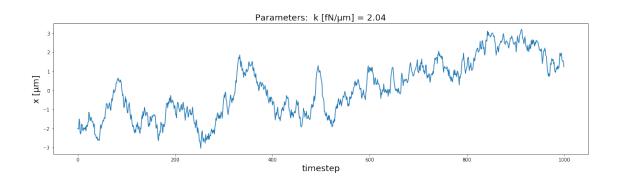


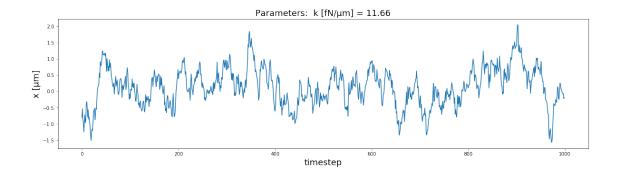


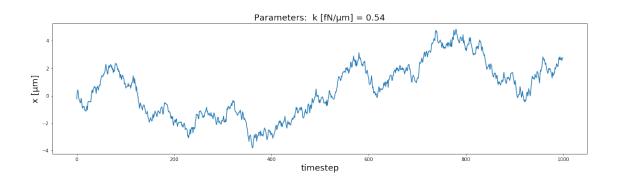


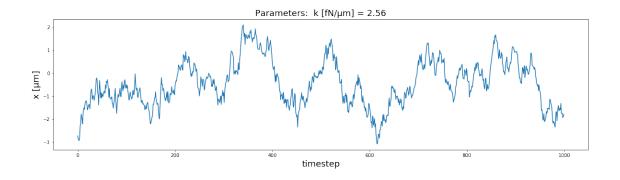


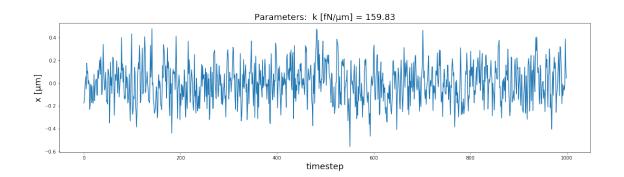












1.4 4. CREATE AND COMPILE DEEP LEARNING NETWORK

The parameters of the deep learning network are defined and the network created. The summary of the network is printed where the output shape and number of parameters for each layer can be visualized.

Comments: 1. The parameter input_shape determines the shape of the input sequence, given by the number of time-steps times the number of samples in each input sequence. Make sure your input shape dimensions match the length of the input trajectory, in this example $2 \times 500 = 1000$. 2. The parameter conv_layers_dimensions determines the number and size of LSTM layers. 3. The parameter number_of_outputs determines the number of outputs, i.e. the number of force field parameters to be estimated.

```
In [6]: ### Define parameters of the deep learning network
    input_shape = (20, 50)
    lstm_layers_dimensions = (1000, 250, 50)
    number_of_outputs = 1

### Create deep learning network
    network = DeepCalib.create_deep_learning_network(input_shape, lstm_layers_dimensions, number_of_output_shape)
### Print deep learning network summary
    network.summary()
```

Layer (type)	Output Shape	Param #
lstm_1 (LSTM)	(None, 20, 1000)	4204000
lstm_2 (LSTM)	(None, 20, 250)	1251000
lstm_3 (LSTM)	(None, 50)	60200
output (Dense)	(None, 1)	51

Total params: 5,515,251 Trainable params: 5,515,251 Non-trainable params: 0

1.5 5. TRAIN DEEP LEARNING NETWORK

The parameters for the training of the deep learning network are defined and the network is trained. The sample size, iteration number, MSE, MAE and the time of each iteration is printed.

Comments: 1. The parameter sample_sizes determines the sizes of the batches of trajectories used in the training. 2. The parameter iteration_numbers determines the numbers of batches used

in the training. 3. The parameter verbose determines the frequency of the update messages. It can be either a boolean value (True/False) or a number between 0 and 1.

```
In [7]: ### Define parameters of the training
        sample_sizes = (32, 128, 512, 2048)
        iteration_numbers = (1001, 1001, 1001, 2001)
        verbose = .1
        ### Training
        training_history = DeepCalib.train_deep_learning_network(network, simulate_trajectory, s
                 32
                                                  MSE
                                                          3.4480
                                                                    MAE
                                                                             1.5706
                                                                                      Time 4950.63829
Sample size
                      iteration number
                                             1
Sample size
                 32
                      iteration number
                                            11
                                                  MSE
                                                          0.7324
                                                                    MAE
                                                                             0.7497
                                                                                      Time 107.949018
                 32
                                             21
                                                  MSE
                                                                                      Time 106.871605
Sample size
                      iteration number
                                                          0.4827
                                                                    MAE
                                                                             0.5501
Sample size
                 32
                      iteration number
                                            31
                                                  MSE
                                                          0.4117
                                                                    MAE
                                                                             0.5009
                                                                                      Time 108.043909
                 32
                                                  MSE
                                                          0.2653
                                                                             0.4318
Sample size
                      iteration number
                                            41
                                                                    MAE
                                                                                      Time 116.273880
Sample size
                 32
                      iteration number
                                            51
                                                  MSE
                                                          0.2784
                                                                    MAE
                                                                             0.4105
                                                                                      Time 106.824636
Sample size
                 32
                      iteration number
                                            61
                                                  MSE
                                                          0.2289
                                                                    MAE
                                                                             0.4020
                                                                                      Time 108.572006
                                                  MSE
                 32
                                            71
                                                          0.2677
                                                                    MAE
                                                                             0.3815
                                                                                      Time 113.693476
Sample size
                      iteration number
Sample size
                 32
                      iteration number
                                            81
                                                  MSE
                                                          0.2203
                                                                    MAE
                                                                             0.3974
                                                                                      Time 110.285759
                 32
                                                  MSE
Sample size
                      iteration number
                                            91
                                                          0.1720
                                                                    MAE
                                                                             0.3497
                                                                                      Time 107.877016
Sample size
                 32
                      iteration number
                                           101
                                                  MSE
                                                          0.2022
                                                                    MAE
                                                                             0.3429
                                                                                      Time 109.894753
                 32
                                           111
                                                  MSE
                                                          0.0810
                                                                    MAE
                                                                             0.2347
                                                                                      Time 110.737801
Sample size
                      iteration number
Sample size
                 32
                      iteration number
                                           121
                                                  MSE
                                                          0.3150
                                                                    MAE
                                                                             0.3838
                                                                                      Time 109.421492
                 32
                                           131
                                                  MSE
                                                          0.2613
                                                                    MAE
                                                                             0.4121
                                                                                      Time 109.548330
Sample size
                      iteration number
Sample size
                 32
                                           141
                                                  MSE
                                                          0.3225
                                                                    MAE
                                                                             0.4410
                                                                                      Time 108.907938
                      iteration number
                 32
                                           151
                                                  MSE
                                                          0.2543
                                                                    MAE
                                                                             0.4201
                                                                                      Time 106.597185
Sample size
                      iteration number
                 32
                                                  MSE
                                                                             0.2848
                                                                                      Time 108.760357
Sample size
                                           161
                                                          0.1407
                                                                    MAE
                      iteration number
                 32
                                           171
Sample size
                      iteration number
                                                  MSE
                                                          0.1853
                                                                    MAE
                                                                             0.3121
                                                                                      Time 110.108376
                 32
                      iteration number
                                           181
                                                  MSE
                                                          0.1198
                                                                    MAE
                                                                             0.2759
                                                                                      Time 107.394218
Sample size
Sample size
                 32
                      iteration number
                                           191
                                                  MSE
                                                          0.0936
                                                                    MAE
                                                                             0.2560
                                                                                      Time 105.220556
                                                  MSE
Sample size
                 32
                      iteration number
                                           201
                                                          0.1455
                                                                    MAE
                                                                             0.3112
                                                                                      Time 108.553410
                 32
                                           211
                                                  MSE
                                                                             0.3421
                                                                                      Time 116.151333
Sample size
                      iteration number
                                                          0.1810
                                                                    MAE
                 32
                                           221
                                                  MSE
                                                                             0.2442
Sample size
                      iteration number
                                                          0.1208
                                                                    MAE
                                                                                      Time 106.971264
                                                                                      Time 105.203152
Sample size
                 32
                      iteration number
                                           231
                                                  MSE
                                                          0.1077
                                                                    MAE
                                                                             0.2539
                 32
                                           241
                                                  MSE
                                                          0.2725
                                                                             0.3981
                                                                                      Time 122.049809
Sample size
                      iteration number
                                                                    MAE
                 32
                                           251
                                                  MSE
Sample size
                      iteration number
                                                          0.0668
                                                                    MAE
                                                                             0.2123
                                                                                      Time 107.476711
                 32
                                           261
                                                  MSE
                                                          0.0984
                                                                             0.2435
Sample size
                      iteration number
                                                                    MAE
                                                                                      Time 109.340668
Sample size
                 32
                      iteration number
                                           271
                                                  MSE
                                                          0.1954
                                                                    MAE
                                                                             0.3267
                                                                                      Time 118.575335
                 32
                                           281
                                                  MSE
                                                          0.0741
                                                                             0.2260
                                                                                      Time 106.934071
Sample size
                      iteration number
                                                                    MAE
Sample size
                 32
                                           291
                                                  MSE
                                                                             0.2905
                                                          0.1426
                                                                    MAE
                                                                                      Time 107.014418
                      iteration number
                 32
                                           301
                                                  MSE
                                                          0.2260
                                                                             0.3590
                                                                                      Time 115.519524
Sample size
                      iteration number
                                                                    MAE
                 32
Sample size
                                           311
                                                  MSE
                                                          0.1538
                                                                    MAE
                                                                             0.3042
                                                                                      Time 106.220722
                      iteration number
Sample size
                 32
                      iteration number
                                           321
                                                  MSE
                                                          0.1707
                                                                    MAE
                                                                             0.3262
                                                                                      Time 108.341217
Sample size
                 32
                      iteration number
                                           331
                                                  MSE
                                                          0.1702
                                                                    MAE
                                                                             0.2855
                                                                                      Time 111.816883
                 32
                                           341
                                                  MSE
                                                          0.2863
                                                                    MAE
                                                                             0.3770
Sample size
                      iteration number
                                                                                      Time 116.181612
Sample size
                 32
                      iteration number
                                           351
                                                  MSE
                                                          0.0703
                                                                    MAE
                                                                             0.1915
                                                                                      Time 107.507944
```

361

MSE

0.0644

MAE

0.1929

Sample size

32

iteration number

Time 111.064434

~ -	•	0.0		-	074	ман	0 1000	360	0.0004	m·	405 540075
Sample		32	iteration		371	MSE	0.1068	MAE	0.2621		105.543375
Sample		32	iteration		381	MSE	0.3928	MAE	0.4599		110.954762
Sample	size	32	iteration	number	391	MSE	0.0798	MAE	0.2302		113.655806
Sample	size	32	iteration	number	401	MSE	0.0702	MAE	0.2217	Time	112.026453
Sample	size	32	iteration	number	411	MSE	0.2004	MAE	0.3760	Time	107.377529
Sample	size	32	iteration	number	421	MSE	0.1245	MAE	0.2531	Time	107.088566
Sample	size	32	iteration	number	431	MSE	0.1596	MAE	0.2880	Time	107.078552
Sample	size	32	iteration	number	441	MSE	0.1346	MAE	0.2498	Time	105.911970
Sample	size	32	iteration	number	451	MSE	0.1667	MAE	0.3348	Time	111.217260
Sample		32	iteration	number	461	MSE	0.2288	MAE	0.2618	Time	108.930349
Sample		32	iteration		471	MSE	0.1270	MAE	0.2411		107.630014
Sample		32	iteration		481	MSE	0.0726	MAE	0.2209		109.687090
Sample		32	iteration		491	MSE	0.2139	MAE	0.3157		106.511116
Sample		32	iteration		501	MSE	0.1325	MAE	0.2701		107.081652
Sample		32	iteration		511	MSE	0.4703	MAE	0.4626		107.785225
Sample		32	iteration		521	MSE	0.1792	MAE	0.2970		112.086535
Sample		32	iteration		531	MSE	0.3006	MAE	0.3322		114.791632
Sample		32	iteration		541	MSE	0.1036	MAE	0.2244		107.793093
Sample		32	iteration		551	MSE	0.2383	MAE	0.3171		113.776207
Sample		32	iteration		561	MSE	0.0936	MAE	0.2204		115.770207
_		32	iteration		571	MSE	0.0930	MAE	0.2204		105.851650
Sample		32	iteration		581	MSE	0.1378	MAE	0.3119		103.031030
Sample						MSE					107.020376
Sample		32	iteration		591		0.1283	MAE	0.2441		
Sample		32	iteration		601	MSE	0.1160	MAE	0.2812		108.039141
Sample		32	iteration		611	MSE	0.0887	MAE	0.2190		107.561111
Sample		32	iteration		621	MSE	0.0927	MAE	0.2252		112.647533
Sample		32	iteration		631	MSE	0.1101	MAE	0.2392		108.156919
Sample		32	iteration		641	MSE	0.1916	MAE	0.3206		109.099150
Sample		32	iteration		651	MSE	0.1531	MAE	0.2700		109.302759
Sample		32	iteration		661	MSE	0.1049	MAE	0.2385		104.348421
Sample		32	iteration		671	MSE	0.0299	MAE	0.1383		106.510401
Sample	size	32	iteration	number	681	MSE	0.1883	MAE	0.2905		106.752157
Sample	size	32	iteration	number	691	MSE	0.1436	MAE	0.2814	Time	106.723547
Sample	size	32	iteration	number	701	MSE	0.0733	MAE	0.1861	Time	108.959913
Sample	size	32	iteration	number	711	MSE	0.1747	MAE	0.2905	Time	113.890409
Sample	size	32	iteration	number	721	MSE	0.1615	MAE	0.2808	Time	105.839729
Sample	size	32	iteration	number	731	MSE	0.1269	MAE	0.2876	Time	107.475996
Sample	size	32	iteration	number	741	MSE	0.2117	MAE	0.3445	Time	107.527971
Sample	size	32	iteration	number	751	MSE	0.0941	MAE	0.2353	Time	113.234520
Sample	size	32	iteration	number	761	MSE	0.1845	MAE	0.2935	Time	112.207651
Sample		32	iteration	number	771	MSE	0.1603	MAE	0.3034		108.115435
Sample		32	iteration		781	MSE	0.1129	MAE	0.2696		108.979940
Sample		32	iteration		791	MSE	0.0841	MAE	0.2274		118.249416
Sample		32	iteration		801	MSE	0.0925	MAE	0.2195		110.401154
Sample		32	iteration		811	MSE	0.1218	MAE	0.2482		108.787537
Sample		32	iteration		821	MSE	0.1946	MAE	0.2644		114.778996
Sample		32	iteration		831	MSE	0.1683	MAE	0.2886		109.090805
Sample		32	iteration		841	MSE	0.1127	MAE	0.2614		109.374046
rambre	DITC	02	1001 a010II	TI OTHING I	041	поп	0.1121	IIAL	0.2014	TIME	100.014040

Sample	size	32	iteration	number	851	MSE	0.1481	MAE	0.3125	Time	108.285189
Sample	size	32	iteration	number	861	MSE	0.1077	MAE	0.2423	Time	109.073400
Sample	size	32	iteration	number	871	MSE	0.1397	MAE	0.2552	Time	103.258371
Sample	size	32	iteration	number	881	MSE	0.2482	MAE	0.3395	Time	107.571125
Sample	size	32	iteration	number	891	MSE	0.0746	MAE	0.1986	Time	107.233047
Sample	size	32	iteration	number	901	MSE	0.0967	MAE	0.2416	Time	107.018471
Sample	size	32	iteration	number	911	MSE	0.0741	MAE	0.2244	Time	105.915546
Sample	size	32	iteration	number	921	MSE	0.1374	MAE	0.2800	Time	108.154058
Sample	size	32	iteration	number	931	MSE	0.2307	MAE	0.3420	Time	107.156754
Sample	size	32	iteration	number	941	MSE	0.1204	MAE	0.2526	Time	107.789993
Sample	size	32	iteration	number	951	MSE	0.1094	MAE	0.2514	Time	109.695196
Sample	size	32	iteration	number	961	MSE	0.2251	MAE	0.2591	Time	105.753660
Sample	size	32	iteration	number	971	MSE	0.1058	MAE	0.2238	Time	104.228258
Sample	size	32	iteration	number	981	MSE	0.0774	MAE	0.2261	Time	105.931520
Sample	size	32	iteration	number	991	MSE	0.0825	MAE	0.2228	Time	109.480858
Sample	size	32	iteration	number	1001	MSE	0.0977	MAE	0.2121	Time	108.372927
Sample	size	128	iteration	number	1	MSE	0.0809	MAE	0.2019	Time	157.453299
Sample	size	128	iteration	number	11	MSE	0.1072	MAE	0.2443	Time	155.901432
Sample	size	128	iteration	number	21	MSE	0.1506	MAE	0.2715	Time	157.845497
Sample	size	128	iteration	number	31	MSE	0.0922	MAE	0.2213	Time	155.067921
Sample	size	128	iteration	number	41	MSE	0.1191	MAE	0.2405	Time	153.770447
Sample	size	128	iteration	number	51	MSE	0.1218	MAE	0.2167	Time	153.401613
Sample	size	128	iteration	number	61	MSE	0.1066	MAE	0.2402	Time	155.587196
Sample	size	128	${\tt iteration}$	number	71	MSE	0.1173	MAE	0.2194	Time	154.132366
Sample	size	128	${\tt iteration}$	number	81	MSE	0.1391	MAE	0.2572	Time	154.666662
Sample	size	128	iteration	number	91	MSE	0.0918	MAE	0.2166	Time	160.052538
Sample	size	128	iteration	number	101	MSE	0.0860	MAE	0.2041	Time	154.836655
Sample	size	128	${\tt iteration}$	number	111	MSE	0.1046	MAE	0.2127	Time	160.001755
Sample	size	128	${\tt iteration}$	number	121	MSE	0.0940	MAE	0.2263	Time	160.674572
Sample	size	128	iteration	number	131	MSE	0.1440	MAE	0.2525	Time	153.858185
Sample	size	128	iteration	number	141	MSE	0.1089	MAE	0.2378	Time	157.707691
Sample	size	128	iteration	number	151	MSE	0.1286	MAE	0.2546	Time	156.742096
Sample	size	128	iteration	number	161	MSE	0.1377	MAE	0.2395	Time	156.768799
Sample	size	128	iteration	number	171	MSE	0.1236	MAE	0.2261	Time	155.079126
Sample	size	128	${\tt iteration}$	number	181	MSE	0.1757	MAE	0.2867	Time	151.708126
Sample	size	128	${\tt iteration}$	number	191	MSE	0.1548	MAE	0.2416	Time	161.392927
Sample	size	128	iteration	number	201	MSE	0.0870	MAE	0.2202	Time	153.826714
Sample	size	128	iteration	number	211	MSE	0.0882	MAE	0.2182	Time	152.835131
Sample	size	128	iteration	number	221	MSE	0.1290	MAE	0.2448	Time	159.835100
Sample	size	128	${\tt iteration}$	number	231	MSE	0.0911	MAE	0.2162	Time	153.860331
Sample	size	128	${\tt iteration}$	number	241	MSE	0.0968	MAE	0.2276	Time	155.947924
Sample	size	128	${\tt iteration}$	number	251	MSE	0.1009	MAE	0.2292	Time	153.896809
Sample	size	128	${\tt iteration}$	number	261	MSE	0.0979	MAE	0.2124	Time	154.290199
Sample	size	128	${\tt iteration}$	number	271	MSE	0.0960	MAE	0.2161	Time	153.170586
Sample	size	128	${\tt iteration}$	number	281	MSE	0.0967	MAE	0.2016		153.917789
Sample	size	128	${\tt iteration}$	number	291	MSE	0.1127	MAE	0.2069	Time	156.054258
Sample	size	128	${\tt iteration}$	number	301	MSE	0.0881	MAE	0.1954	Time	155.501842
Sample	size	128	${\tt iteration}$	number	311	MSE	0.1757	MAE	0.2747	Time	156.705379

Sample	size	128	iteration	number	321	MSE	0.0808	MAE	0.2081	Time	155.234575
Sample	size	128	iteration	number	331	MSE	0.1048	MAE	0.2251	Time	158.791542
Sample	size	128	iteration	number	341	MSE	0.1286	MAE	0.2569	Time	153.782129
Sample	size	128	iteration	number	351	MSE	0.1227	MAE	0.2469	Time	157.235622
Sample	size	128	iteration	number	361	MSE	0.1678	MAE	0.2937	Time	154.797792
Sample	size	128	iteration	number	371	MSE	0.0872	MAE	0.2137	Time	155.803919
Sample	size	128	iteration	number	381	MSE	0.1222	MAE	0.2270	Time	154.669046
Sample	size	128	iteration	number	391	MSE	0.1319	MAE	0.2439	Time	155.096292
Sample	size	128	iteration	number	401	MSE	0.1107	MAE	0.2327	Time	154.300928
Sample	size	128	iteration	number	411	MSE	0.1247	MAE	0.2396	Time	162.825346
Sample	size	128	iteration	number	421	MSE	0.1065	MAE	0.2399	Time	155.696869
Sample	size	128	iteration	number	431	MSE	0.1166	MAE	0.2227	Time	154.034853
Sample		128	iteration	number	441	MSE	0.1114	MAE	0.2336	Time	153.184891
Sample		128	iteration		451	MSE	0.0781	MAE	0.1858		155.972242
Sample		128	iteration		461	MSE	0.1471	MAE	0.2461		156.067610
Sample		128	iteration		471	MSE	0.1287	MAE	0.2593		167.557240
Sample		128	iteration		481	MSE	0.1130	MAE	0.2422		155.010223
Sample		128	iteration		491	MSE	0.1016	MAE	0.2086		164.391518
Sample		128	iteration		501	MSE	0.1662	MAE	0.2774		155.107975
Sample		128	iteration		511	MSE	0.1187	MAE	0.2419		154.377699
Sample		128	iteration		521	MSE	0.1053	MAE	0.2248		163.006067
Sample		128	iteration		531	MSE	0.1095	MAE	0.2367		152.789831
Sample		128	iteration		541	MSE	0.1160	MAE	0.2410		154.630184
Sample		128	iteration		551	MSE	0.1358	MAE	0.2542		153.218985
Sample		128	iteration		561	MSE	0.1385	MAE	0.2392		163.444996
Sample		128	iteration		571	MSE	0.1078	MAE	0.2436		153.837919
Sample		128	iteration		581	MSE	0.1439	MAE	0.2561		166.818142
Sample		128	iteration		591	MSE	0.1327	MAE	0.2315		156.110287
Sample		128	iteration		601	MSE	0.1090	MAE	0.2353		153.063774
Sample		128	iteration		611	MSE	0.0839	MAE	0.1945		158.921957
Sample		128	iteration		621	MSE	0.1008	MAE	0.2277		157.111168
Sample		128	iteration		631	MSE	0.1444	MAE	0.2579		150.013208
Sample		128	iteration		641	MSE	0.1196	MAE	0.2253		156.994820
Sample		128	iteration		651	MSE	0.0928	MAE	0.1994		155.798912
Sample		128 128	iteration iteration		661 671	MSE MSE	0.0986 0.0833	MAE	0.2203 0.2073		152.577877 156.449080
Sample Sample		128	iteration		681	MSE	0.0835	MAE MAE	0.2073		154.718161
Sample		128	iteration		691	MSE	0.0823	MAE	0.1984		151.053905
Sample		128	iteration		701	MSE	0.0342	MAE	0.2128		166.045189
Sample		128	iteration		711	MSE	0.1657	MAE	0.1567		156.754255
Sample		128	iteration		721	MSE	0.1037	MAE	0.2352		161.048174
Sample		128	iteration		731	MSE	0.1118	MAE	0.1903		155.667782
Sample		128	iteration		741	MSE	0.0009	MAE	0.1903		155.841589
Sample		128	iteration		751	MSE	0.0742	MAE	0.2306		154.063702
Sample		128	iteration		761	MSE	0.1076	MAE	0.2431		150.608301
Sample		128	iteration		771	MSE	0.0989	MAE	0.2225		156.491041
Sample		128	iteration		781	MSE	0.1132	MAE	0.2321		156.325340
Sample		128	iteration		791	MSE	0.1017	MAE	0.2291		158.656836
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Sample	size	128	iteration	number	801	MSE	0.1104	MAE	0.2362	Time	160.16936
Sample	size	128	iteration	number	811	MSE	0.1158	MAE	0.2390	Time	156.91161
Sample	size	128	iteration	number	821	MSE	0.1205	MAE	0.2464	Time	157.25374
Sample	size	128	iteration	number	831	MSE	0.1016	MAE	0.2435	Time	157.30905
Sample	size	128	iteration	number	841	MSE	0.0790	MAE	0.1991	Time	154.81925
Sample		128	iteration	number	851	MSE	0.1583	MAE	0.2702	Time	152.56786
Sample		128	iteration	number	861	MSE	0.1237	MAE	0.2465	Time	157.10687
Sample		128	iteration	number	871	MSE	0.1066	MAE	0.2115	Time	155.02309
Sample		128	iteration	number	881	MSE	0.0851	MAE	0.2062	Time	160.37011
Sample		128	iteration	number	891	MSE	0.1013	MAE	0.2232	Time	158.12468
Sample	size	128	iteration	number	901	MSE	0.0924	MAE	0.2125	Time	156.08978
Sample		128	iteration	number	911	MSE	0.1412	MAE	0.2564	Time	153.94020
Sample		128	iteration	number	921	MSE	0.1140	MAE	0.2145		152.60052
Sample		128	iteration	number	931	MSE	0.0884	MAE	0.2073		151.20601
Sample		128	iteration	number	941	MSE	0.1161	MAE	0.2294	Time	152.05955
Sample		128	iteration	number	951	MSE	0.0985	MAE	0.2131		156.21542
Sample		128	iteration		961	MSE	0.1006	MAE	0.2109		154.98352
Sample		128	iteration		971	MSE	0.1333	MAE	0.2602	Time	156.40449
Sample	size	128	iteration	number	981	MSE	0.1094	MAE	0.2246	Time	157.83286
Sample	size	128	iteration	number	991	MSE	0.0948	MAE	0.2075	Time	163.28454
Sample		128	iteration	number	1001	MSE	0.0603	MAE	0.1764	Time	155.28941
Sample	size	512	iteration	number	1	MSE	0.1189	MAE	0.2339	Time	354.24661
Sample	size	512	iteration	number	11	MSE	0.1150	MAE	0.2153	Time	345.41201
Sample	size	512	iteration	number	21	MSE	0.1108	MAE	0.2199	Time	343.70803
Sample	size	512	iteration	number	31	MSE	0.1228	MAE	0.2353	Time	350.22163
Sample	size	512	iteration	number	41	MSE	0.0886	MAE	0.2053	Time	348.92344
Sample	size	512	iteration	number	51	MSE	0.1170	MAE	0.2380	Time	354.82001
Sample	size	512	iteration	number	61	MSE	0.1275	MAE	0.2327	Time	350.62122
Sample	size	512	iteration	number	71	MSE	0.0929	MAE	0.2035	Time	348.69098
Sample	size	512	iteration	number	81	MSE	0.1175	MAE	0.2262	Time	352.14543
Sample	size	512	iteration	number	91	MSE	0.1124	MAE	0.2348	Time	348.11830
Sample	size	512	iteration	number	101	MSE	0.1078	MAE	0.2197	Time	346.41003
Sample	size	512	iteration	number	111	MSE	0.1079	MAE	0.2206	Time	349.86138
Sample	size	512	iteration	number	121	MSE	0.0857	MAE	0.2025	Time	349.28083
Sample	size	512	iteration	number	131	MSE	0.1107	MAE	0.2224	Time	340.24977
Sample	size	512	iteration	number	141	MSE	0.1053	MAE	0.2150	Time	342.71836
Sample	size	512	iteration	number	151	MSE	0.0957	MAE	0.2124	Time	347.78618
Sample		512	iteration	number	161	MSE	0.1010	MAE	0.2109	Time	348.65236
Sample	size	512	iteration	number	171	MSE	0.0903	MAE	0.2015	Time	349.75767
Sample		512	iteration	number	181	MSE	0.1038	MAE	0.2213	Time	354.75468
Sample	size	512	iteration	number	191	MSE	0.1015	MAE	0.2172	Time	347.75042
Sample		512	iteration	number	201	MSE	0.1220	MAE	0.2336	Time	357.28240
Sample		512	iteration	number	211	MSE	0.1286	MAE	0.2401	Time	362.96844
Sample		512	iteration	number	221	MSE	0.1176	MAE	0.2330	Time	349.03621
Sample		512	iteration	number	231	MSE	0.1137	MAE	0.2154	Time	346.29583
Sample		512	iteration	number	241	MSE	0.1054	MAE	0.2250	Time	354.05159
Sample		512	iteration	number	251	MSE	0.1213	MAE	0.2358	Time	353.16300
Sample		512	iteration	number	261	MSE	0.1097	MAE	0.2210	Time	361.49954
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Sample size 512 iteration number 221 MSE 0.1014 MAE 0.2193 Time 351,3832 Sample size 512 iteration number 291 MSE 0.042 MAE 0.2295 Time 354,0496 Sample size 512 iteration number 301 MSE 0.0829 MAE 0.2234 Time 360,12387 Sample size 512 iteration number 321 MSE 0.1077 MAE 0.2203 Time 360,12387 Sample size 512 iteration number 331 MSE 0.1077 MAE 0.2208 Time 351,9476 Sample size 512 iteration number 351 MSE 0.1003 MAE 0.2179 Time 341,96281 Sample size 512 iteration number 351 MSE 0.1063 MAE 0.2219 Time 349,3618 Sample size 512 iteration number 361 MSE 0.1063 MAE 0.2207 Time 349,3618 Sample size 512 iteration n													
Sample size 512 iteration number 291 MSE 0.1135 MAE 0.2295 Time 357.74588 Sample size 512 iteration number 301 MSE 0.1278 MAE 0.2203 Time 367.74588 Sample size 512 iteration number 311 MSE 0.1077 MAE 0.2208 Time 361.94754 Sample size 512 iteration number 311 MSE 0.1063 MAE 0.2079 Time 364.22965 Sample size 512 iteration number 351 MSE 0.1100 MAE 0.2279 Time 364.2968 Sample size 512 iteration number 361 MSE 0.1106 MAE 0.2279 Time 349.3618 Sample size 512 iteration number 371 MSE 0.1040 MAE 0.2207 Time 349.3618 Sample size 512 iteration number 401 MSE 0.1046 MAE 0.2217 Time 357.65560 Sample size 512 iteratio	Sample	size	512	iteration	number	271	MSE	0.1101	MAE	0.2123	Time	351.383	209
Sample size 512 iteration number 301 MSE 0.0929 MAE 0.2018 Time 357.74586 Sample size 512 iteration number 311 MSE 0.1278 MAE 0.2324 Time 360.12387 Sample size 512 iteration number 331 MSE 0.1077 MAE 0.2008 Time 351.94568 Sample size 512 iteration number 331 MSE 0.1013 MAE 0.2070 Time 361.22954 Sample size 512 iteration number 341 MSE 0.1063 MAE 0.2079 Time 341.96281 Sample size 512 iteration number 361 MSE 0.1110 MAE 0.2207 Time 348.03403 Sample size 512 iteration number 361 MSE 0.1110 MAE 0.2207 Time 349.3611 Sample size 512 iteration number 381 MSE 0.1146 MAE 0.2207 Time 349.3612 Sample size 512 iteration number 381 MSE 0.1148 MAE 0.2205 Time 349.3613 Sample size 512 iteration number 381 MSE 0.0161 MAE 0.2207 Time 349.3613 Sample size 512 iteration number 401 MSE 0.0980 MAE 0.2093 Time 357.67456 Sample size 512 iteration number 411 MSE 0.0980 MAE 0.2016 Time 357.67456 Sample size 512 iteration number 421 MSE 0.0980 MAE 0.2161 Time 357.67456 Sample size 512 iteration number 441 MSE 0.0980 MAE 0.2161 Time 357.67456 Sample size 512 iteration number 441 MSE 0.0980 MAE 0.2161 Time 359.39407 Sample size 512 iteration number 441 MSE 0.0980 MAE 0.2161 Time 359.39407 Sample size 512 iteration number 441 MSE 0.1075 MAE 0.2144 Time 353.12967 Sample size 512 iteration number 441 MSE 0.1075 MAE 0.2141 Time 359.39307 Sample size 512 iteration number 451 MSE 0.1075 MAE 0.2141 Time 359.39307 Sample size 512 iteration number 451 MSE 0.1075 MAE 0.2141 Time 377.89831 MSE 0.1082 MAE 0.2141 Time 377.89831 MSE 0.1082 MAE 0.2141 Time 377.89831 MSE 0.1082 MAE 0.2161 Time 377.89831 MSE 0.1082 MAE 0.2161 Time 377.89831 MSE 0.1082 MAE	Sample	size	512	iteration	number	281	MSE	0.1042	MAE	0.2093	Time	354.269	266
Sample size 512 iteration number 311 MSE 0.1278 MAE 0.2324 Time 360.12367 Sample size 512 iteration number 321 MSE 0.1077 MAE 0.2208 Time 351.94754 Sample size 512 iteration number 341 MSE 0.1063 MAE 0.2279 Time 361.9287 Sample size 512 iteration number 361 MSE 0.1160 MAE 0.2207 Time 361.9628 Sample size 512 iteration number 361 MSE 0.1166 MAE 0.2207 Time 361.9383 Sample size 512 iteration number 361 MSE 0.1166 MAE 0.2273 Time 341.9284 Sample size 512 iteration number 391 MSE 0.1037 MAE 0.203 Time 345.1294 Sample size 512 iteration number 401 MSE 0.0808 MAE 0.2161 Time 356.0926 Sample size 512 iteration nu	Sample	size	512	iteration	number	291	MSE	0.1135	MAE	0.2295	Time	354.049	383
Sample size 512 iteration number 321 MSE 0.0917 MAE 0.2070 Time 351.94754 Sample size 512 iteration number 341 MSE 0.1913 MAE 0.2070 Time 356.22954 Sample size 512 iteration number 341 MSE 0.1110 MAE 0.2208 Time 351.14526 Sample size 512 iteration number 361 MSE 0.1110 MAE 0.2208 Time 351.14526 Sample size 512 iteration number 361 MSE 0.1116 MAE 0.2208 Time 351.14526 Sample size 512 iteration number 371 MSE 0.1166 MAE 0.2209 Time 349.36118 Sample size 512 iteration number 371 MSE 0.1037 MAE 0.2205 Time 345.12946 Sample size 512 iteration number 371 MSE 0.1016 MAE 0.2225 Time 345.12946 Sample size 512 iteration number 401 MSE 0.1016 MAE 0.2212 Time 350.90470 Sample size 512 iteration number 411 MSE 0.0980 MAE 0.2212 Time 350.90470 Sample size 512 iteration number 431 MSE 0.0980 MAE 0.2212 Time 350.90470 Sample size 512 iteration number 431 MSE 0.0989 MAE 0.2214 Time 354.14457 Sample size 512 iteration number 441 MSE 0.0989 MAE 0.2214 Time 354.34457 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2214 Time 352.98016 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2214 Time 352.89016 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2144 Time 353.12966 Sample size 512 iteration number 471 MSE 0.1024 MAE 0.2130 Time 347.58938 Sample size 512 iteration number 481 MSE 0.1075 MAE 0.2130 Time 347.58938 Sample size 512 iteration number 481 MSE 0.1075 MAE 0.2130 Time 347.58938 Sample size 512 iteration number 511 MSE 0.1075 MAE 0.2208 Time 345.56082 Sample size 512 iteration number 511 MSE 0.1075 MAE 0.2208 Time 345.56082 Sample size 512 iteration number 511 MSE 0.1076 MAE 0.22	Sample	size	512	iteration	number	301	MSE	0.0929	MAE	0.2018	Time	357.745	386
Sample size 512 iteration number 331 MSE 0.0913 MAE 0.2070 Time 366.22954 Sample size 512 iteration number 361 MSE 0.1063 MAE 0.2179 Time 341.96281 Sample size 512 iteration number 361 MSE 0.1160 MAE 0.2208 Time 341.96281 Sample size 512 iteration number 361 MSE 0.1037 MAE 0.2279 Time 348.30403 Sample size 512 iteration number 361 MSE 0.1037 MAE 0.2279 Time 348.30403 Sample size 512 iteration number 361 MSE 0.1037 MAE 0.2212 Time 349.36118 Sample size 512 iteration number 361 MSE 0.1037 MAE 0.2203 Time 357.65504 Sample size 512 iteration number 401 MSE 0.0980 MAE 0.2203 Time 357.65504 Sample size 512 iteration number 411 MSE 0.0980 MAE 0.2212 Time 350.9047 Sample size 512 iteration number 421 MSE 0.0987 MAE 0.2016 Time 357.67458 Sample size 512 iteration number 431 MSE 0.0989 MAE 0.2016 Time 344.20015 Sample size 512 iteration number 441 MSE 0.0744 MAE 0.2016 Time 344.20015 Sample size 512 iteration number 441 MSE 0.1075 MAE 0.2273 Time 352.93607 Sample size 512 iteration number 451 MSE 0.1075 MAE 0.2273 Time 352.93608 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2141 Time 358.31296 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2141 Time 358.31296 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2141 Time 358.31296 Sample size 512 iteration number 461 MSE 0.1075 MAE 0.2141 Time 356.0822 Sample size 512 iteration number 501 MSE 0.1075 MAE 0.2103 Time 347.18799 Sample size 512 iteration number 501 MSE 0.1075 MAE 0.2208 Time 346.18905 Sample size 512 iteration number 501 MSE 0.1060 MAE 0.2207 Time 346.19905 Sample size 512 iteration number 501 MSE 0.1075 MAE 0.2207 Time 346.19905 Sample size 512 it	Sample	size	512	iteration	number	311	MSE	0.1278	MAE	0.2324	Time	360.123	373
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Sample size 512 iteration number 701 MSE 0.1095 MAE 0.2205 Time 355.47375 Sample size 512 iteration number 711 MSE 0.0915 MAE 0.2084 Time 356.57358 Sample size 512 iteration number 721 MSE 0.1016 MAE 0.2187 Time 352.11706 Sample size 512 iteration number 731 MSE 0.1123 MAE 0.2252 Time 348.99640	_												
Sample size 512 iteration number 711 MSE 0.0915 MAE 0.2084 Time 356.57358 Sample size 512 iteration number 721 MSE 0.1016 MAE 0.2187 Time 352.11706 Sample size 512 iteration number 731 MSE 0.1123 MAE 0.2252 Time 348.99640	_												
Sample size 512 iteration number 721 MSE 0.1016 MAE 0.2187 Time 352.11706 Sample size 512 iteration number 731 MSE 0.1123 MAE 0.2252 Time 348.99640	=												
Sample size 512 iteration number 731 MSE 0.1123 MAE 0.2252 Time 348.99640	· =												
	=			iteration	number	731	MSE	0.1123					
	=		512	iteration	number	741	MSE	0.0944	MAE	0.2102	Time	359.152	317

Sample	size	512	iteration	number	751	MSE	0.1099	MAE	0.2161	Time	353.363	3991
Sample	size	512	iteration	number	761	MSE	0.1127	MAE	0.2169	Time	345.863	3581
Sample	size	512	iteration	number	771	MSE	0.0950	MAE	0.2183	Time	353.57	5468
Sample	size	512	iteration	number	781	MSE	0.1151	MAE	0.2291	Time	349.410	0295
Sample		512	iteration	number	791	MSE	0.1110	MAE	0.2211	Time	350.28	4100
Sample		512	iteration		801	MSE	0.1035	MAE	0.2154		359.10	
Sample		512	iteration		811	MSE	0.1160	MAE	0.2238		361.73	
Sample		512	iteration		821	MSE	0.1082	MAE	0.2211		346.38	
Sample		512	iteration		831	MSE	0.1081	MAE	0.2154		349.46	
Sample		512	iteration		841	MSE	0.1047	MAE	0.2218		346.148	
Sample		512	iteration		851	MSE	0.1150	MAE	0.2251		348.840	
Sample		512	iteration	number	861	MSE	0.1030	MAE	0.2183		367.92	
Sample		512	iteration		871	MSE	0.1009	MAE	0.2253		371.340	
Sample		512	iteration	number	881	MSE	0.1121	MAE	0.2241	Time	344.470	0739
Sample		512	iteration	number	891	MSE	0.1227	MAE	0.2320	Time	347.89	5861
Sample	size	512	iteration	number	901	MSE	0.1139	MAE	0.2223	Time	364.10	9278
Sample		512	iteration	number	911	MSE	0.1072	MAE	0.2175	Time	345.03	2930
Sample		512	iteration	number	921	MSE	0.1154	MAE	0.2302	Time	347.34	1776
Sample		512	iteration	number	931	MSE	0.1064	MAE	0.2098	Time	352.18	7872
Sample		512	iteration	number	941	MSE	0.1110	MAE	0.2242	Time	351.80	4495
Sample		512	iteration	number	951	MSE	0.1012	MAE	0.2192	Time	347.59	2354
Sample	size	512	iteration	number	961	MSE	0.1140	MAE	0.2217	Time	347.56	1836
Sample	size	512	iteration	number	971	MSE	0.0888	MAE	0.2044	Time	360.013	3723
Sample		512	iteration	number	981	MSE	0.1071	MAE	0.2219	Time	356.43	6729
Sample		512	iteration	number	991	MSE	0.1099	MAE	0.2266	Time	347.20	7069
Sample		512	iteration	number	1001	MSE	0.0918	MAE	0.2097	Time	354.120	0731
Sample		2048	iteration	number	1	MSE	0.1150	MAE	0.2207	Time	1097.8	7917
Sample		2048	iteration	number	11	MSE	0.1062	MAE	0.2165	Time	1097.5	1915
Sample		2048	iteration	number	21	MSE	0.1092	MAE	0.2183	Time	1093.7	500d
Sample	size	2048	iteration	number	31	MSE	0.0965	MAE	0.2026	Time	1183.1	5792
Sample	size	2048	iteration	number	41	MSE	0.1064	MAE	0.2168	Time	1114.50	0696
Sample	size	2048	iteration	number	51	MSE	0.1010	MAE	0.2104	Time	1088.00	0125
Sample	size	2048	iteration	number	61	MSE	0.1052	MAE	0.2133	Time	1084.5	1628
Sample		2048	iteration	number	71	MSE	0.1067	MAE	0.2160	Time	1098.3	3598
Sample		2048	iteration	number	81	MSE	0.1067	MAE	0.2148	Time	1112.2	5175
Sample	size	2048	iteration	number	91	MSE	0.1105	MAE	0.2245	Time	1103.3	1344
Sample	size	2048	iteration	number	101	MSE	0.1094	MAE	0.2199	Time	1096.8	1367
Sample	size	2048	iteration	number	111	MSE	0.0984	MAE	0.2105	Time	1096.20	0213
Sample	size	2048	iteration	number	121	MSE	0.0905	MAE	0.1998	Time	1099.9	4936
Sample	size	2048	iteration	number	131	MSE	0.1022	MAE	0.2155	Time	1090.7	6595
Sample		2048	iteration	number	141	MSE	0.1013	MAE	0.2101	Time	1105.2	7634
Sample	size	2048	iteration	number	151	MSE	0.1067	MAE	0.2143	Time	1100.10	0027
Sample	size	2048	iteration	number	161	MSE	0.1006	MAE	0.2140	Time	1099.1	1704
Sample	size	2048	iteration	number	171	MSE	0.1006	MAE	0.2155	Time	1096.8	7495
Sample	size	2048	iteration	number	181	MSE	0.0994	MAE	0.2075	Time	1105.1	4545
Sample	size	2048	iteration	number	191	MSE	0.0947	MAE	0.2034	Time	1092.38	8410
Sample	size	2048	iteration	number	201	MSE	0.1118	MAE	0.2212	Time	1101.8	4001
Sample	size	2048	iteration	number	211	MSE	0.1072	MAE	0.2182	Time	1092.0	5579

Sample	size	2048	iteration	number	221	MSE	0.1058	MAE	0.2154	Time	1100	.03924
Sample	size	2048	iteration	number	231	MSE	0.1104	MAE	0.2170	Time	1091	.43161
Sample	size	2048	iteration	number	241	MSE	0.1033	MAE	0.2184	Time	1093	. 28270
Sample	size	2048	iteration	number	251	MSE	0.1025	MAE	0.2138	Time	1094	. 25377
Sample	size	2048	iteration	number	261	MSE	0.1061	MAE	0.2176	Time	1101	.51410
Sample		2048	iteration	number	271	MSE	0.0935	MAE	0.2077	Time	1093	. 90425
Sample		2048	iteration	number	281	MSE	0.1017	MAE	0.2157	Time	1113	.89184
Sample		2048	iteration	number	291	MSE	0.1065	MAE	0.2174	Time	1097	. 11194
Sample	size	2048	iteration	number	301	MSE	0.1009	MAE	0.2125	Time	1096	.32921
Sample		2048	iteration	number	311	MSE	0.1002	MAE	0.2128	Time	1093	.70064
Sample		2048	iteration	number	321	MSE	0.0942	MAE	0.2073	Time	1100	. 28815
Sample		2048	iteration	number	331	MSE	0.1137	MAE	0.2233			. 96243
Sample		2048	iteration	number	341	MSE	0.1100	MAE	0.2241			. 54087
Sample		2048	iteration	number	351	MSE	0.0999	MAE	0.2131			. 48363
Sample		2048	iteration	number	361	MSE	0.1074	MAE	0.2160	Time	1092	. 15951
Sample		2048	iteration	number	371	MSE	0.0998	MAE	0.2102	Time	1099	.03240
Sample		2048	iteration	number	381	MSE	0.1015	MAE	0.2119			. 56522
Sample		2048	iteration	number	391	MSE	0.1096	MAE	0.2177	Time	1094	. 91396
Sample		2048	iteration	number	401	MSE	0.1095	MAE	0.2215	Time	1100	.89874
Sample		2048	iteration	number	411	MSE	0.1023	MAE	0.2157	Time	1100	.05164
Sample		2048	iteration	number	421	MSE	0.0969	MAE	0.2079	Time	1102	. 19168
Sample		2048	iteration	number	431	MSE	0.0985	MAE	0.2103	Time	1095	.77965
Sample	size	2048	iteration	number	441	MSE	0.1080	MAE	0.2228	Time	1097	. 46980
Sample	size	2048	iteration	number	451	MSE	0.0976	MAE	0.2100	Time	1098	. 36888
Sample	size	2048	iteration	number	461	MSE	0.0993	MAE	0.2140	Time	1103	.45602
Sample	size	2048	iteration	number	471	MSE	0.1040	MAE	0.2170	Time	1101	.65691
Sample	size	2048	iteration	number	481	MSE	0.1088	MAE	0.2195	Time	1097	. 24783
Sample	size	2048	iteration	number	491	MSE	0.0967	MAE	0.2060	Time	1131	. 98638
Sample	size	2048	iteration	number	501	MSE	0.1109	MAE	0.2195	Time	1116	.42432
Sample	size	2048	iteration	number	511	MSE	0.1072	MAE	0.2152	Time	1115	.19956
Sample	size	2048	iteration	number	521	MSE	0.1082	MAE	0.2209	Time	1095	.90411
Sample	size	2048	iteration	number	531	MSE	0.1154	MAE	0.2247	Time	1080	. 25527
Sample	size	2048	iteration	number	541	MSE	0.1144	MAE	0.2280	Time	1084	. 78879
Sample	size	2048	iteration	number	551	MSE	0.0972	MAE	0.2087	Time	1161	.30685
Sample	size	2048	iteration	number	561	MSE	0.1041	MAE	0.2196	Time	1086	.83514
Sample	size	2048	iteration	number	571	MSE	0.1110	MAE	0.2192	Time	1079	.40197
Sample	size	2048	iteration	number	581	MSE	0.1053	MAE	0.2155	Time	1085	. 24537
Sample	size	2048	iteration	number	591	MSE	0.1030	MAE	0.2164	Time	1083	.12702
Sample	size	2048	iteration	number	601	MSE	0.1174	MAE	0.2258	Time	1186	.82241
Sample	size	2048	iteration	number	611	MSE	0.1020	MAE	0.2132	Time	1100	. 48532
Sample	size	2048	iteration	number	621	MSE	0.1095	MAE	0.2165	Time	1091	.06302
Sample	size	2048	${\tt iteration}$	number	631	MSE	0.1066	MAE	0.2149	Time	1084	.49745
Sample	size	2048	${\tt iteration}$	number	641	MSE	0.1045	MAE	0.2114	Time	1090	. 63243
Sample	size	2048	${\tt iteration}$	number	651	MSE	0.1010	MAE	0.2156	Time	1087	.37754
Sample	size	2048	${\tt iteration}$	number	661	MSE	0.1013	MAE	0.2103	Time	1090	. 26813
Sample	size	2048	${\tt iteration}$	number	671	MSE	0.0973	MAE	0.2103	Time	1164	. 64424
Sample		2048	${\tt iteration}$	number	681	MSE	0.1052	MAE	0.2159			. 15294
Sample	size	2048	iteration	number	691	MSE	0.0954	MAE	0.2072	Time	1105	.07154

Sample	size	2048	iteration	number	701	MSE	0.1070	MAE	0.2132	Time	1094.28572
Sample		2048	iteration	number	711	MSE	0.1078	MAE	0.2196		1100.12483
Sample		2048	iteration	number	721	MSE	0.1073	MAE	0.2114	Time	1092.65232
Sample	size	2048	iteration	number	731	MSE	0.1122	MAE	0.2213	Time	1096.46892
Sample		2048	iteration	number	741	MSE	0.1007	MAE	0.2106	Time	1097.63455
Sample		2048	iteration	number	751	MSE	0.0978	MAE	0.2116		1097.43213
Sample		2048	iteration	number	761	MSE	0.1055	MAE	0.2172		1099.09486
Sample		2048	iteration	number	771	MSE	0.1126	MAE	0.2226	Time	1098.81377
Sample		2048	iteration	number	781	MSE	0.0959	MAE	0.2072	Time	1094.04873
Sample	size	2048	iteration	number	791	MSE	0.1035	MAE	0.2114	Time	1100.92711
Sample		2048	iteration	number	801	MSE	0.1079	MAE	0.2154	Time	1121.84619
Sample	size	2048	iteration	number	811	MSE	0.1126	MAE	0.2217	Time	1131.13141
Sample	size	2048	iteration	number	821	MSE	0.1101	MAE	0.2178	Time	1100.23808
Sample	size	2048	iteration	number	831	MSE	0.1013	MAE	0.2115	Time	1098.53744
Sample	size	2048	iteration	number	841	MSE	0.1071	MAE	0.2177	Time	1100.36969
Sample	size	2048	iteration	number	851	MSE	0.1104	MAE	0.2193	Time	1097.55253
Sample	size	2048	iteration	number	861	MSE	0.1005	MAE	0.2079	Time	1098.45399
Sample	size	2048	iteration	number	871	MSE	0.0992	MAE	0.2051	Time	1093.54972
Sample	size	2048	iteration	number	881	MSE	0.1019	MAE	0.2124	Time	1097.35560
Sample	size	2048	iteration	number	891	MSE	0.0984	MAE	0.2063	Time	1096.86803
Sample	size	2048	iteration	number	901	MSE	0.1078	MAE	0.2156	Time	1126.56307
Sample	size	2048	iteration	number	911	MSE	0.1108	MAE	0.2208		1102.98633
Sample	size	2048	${\tt iteration}$	number	921	MSE	0.1001	MAE	0.2103	Time	1105.39364
Sample	size	2048	${\tt iteration}$	number	931	MSE	0.1104	MAE	0.2129	Time	1099.63131
Sample	size	2048	${\tt iteration}$		941	MSE	0.1157	MAE	0.2258	Time	1103.41596
Sample	size	2048	${\tt iteration}$	number	951	MSE	0.1207	MAE	0.2275		1123.12865
Sample	size	2048	iteration		961	MSE	0.1027	MAE	0.2128		1097.27144
Sample		2048	iteration		971	MSE	0.1047	MAE	0.2123		1109.10725
Sample		2048	iteration		981	MSE	0.1225	MAE	0.2243		1107.51223
Sample		2048	iteration		991	MSE	0.1093	MAE	0.2230		1112.69640
Sample		2048	iteration		1001	MSE	0.1002	MAE	0.2139		1096.48251
Sample		2048	iteration		1011	MSE	0.1118	MAE	0.2214		1098.91271
Sample		2048	iteration		1021	MSE	0.1028	MAE	0.2141		1091.45927
Sample		2048	iteration		1031	MSE	0.1067	MAE	0.2153		1090.89541
Sample		2048	iteration		1041	MSE	0.1115	MAE	0.2156		1126.56688
Sample		2048	iteration		1051	MSE	0.1036	MAE	0.2136		1113.55519
Sample		2048	iteration		1061	MSE	0.1012	MAE	0.2044		1108.20937
Sample		2048	iteration		1071	MSE	0.0984	MAE	0.2073		1099.05123
Sample		2048	iteration		1081	MSE	0.0985	MAE	0.2096		1097.87488
Sample		2048	iteration		1091	MSE	0.1101	MAE	0.2190		1098.63591
Sample		2048	iteration		1101	MSE	0.1070	MAE	0.2146		1101.92585
Sample		2048	iteration		1111	MSE	0.1080	MAE	0.2155		1103.01041
Sample		2048	iteration		1121	MSE	0.0971	MAE	0.2132		1107.69176
Sample		2048	iteration		1131	MSE	0.1013	MAE	0.2087		1102.98419
Sample		2048	iteration		1141	MSE	0.0954	MAE	0.2080		1100.64697
Sample		2048	iteration		1151	MSE	0.0972	MAE	0.2076		1099.80154
Sample		2048	iteration		1161	MSE	0.1080	MAE	0.2150		1101.67145
Sample	size	2048	iteration	number	1171	MSE	0.1051	MAE	0.2169	Time	1096.98605

Sample	size	2048	iteration	number	1181	MSE	0.0990	MAE	0.2146	Time	1089	.36071
Sample	size	2048	iteration	number	1191	MSE	0.1016	MAE	0.2119	Time	1091	. 93205
Sample	size	2048	iteration	number	1201	MSE	0.1141	MAE	0.2237	Time	1099	. 65705
Sample	size	2048	iteration	number	1211	MSE	0.0971	MAE	0.2047	Time	1098	.01936
Sample		2048	iteration	number	1221	MSE	0.1062	MAE	0.2167	Time	1095	.72386
Sample		2048	iteration		1231	MSE	0.1021	MAE	0.2112			. 62027
Sample		2048	iteration		1241	MSE	0.1037	MAE	0.2137			. 99668
Sample		2048	iteration		1251	MSE	0.1061	MAE	0.2168			. 16398
Sample		2048	iteration		1261	MSE	0.1102	MAE	0.2174			. 68738
Sample		2048	iteration		1271	MSE	0.1030	MAE	0.2139			.80705
Sample		2048	iteration		1281	MSE	0.1070	MAE	0.2198			. 26172
Sample		2048	iteration		1291	MSE	0.1156	MAE	0.2192			. 58102
Sample		2048	iteration	number	1301	MSE	0.1097	MAE	0.2254			. 98664
Sample		2048	iteration	number	1311	MSE	0.0921	MAE	0.1975			.79207
Sample		2048	iteration	number	1321	MSE	0.1045	MAE	0.2157	Time	1098	.85478
Sample		2048	iteration	number	1331	MSE	0.1035	MAE	0.2153	Time	1094	. 24877
Sample		2048	iteration	number	1341	MSE	0.1036	MAE	0.2154	Time	1103	.91712
Sample		2048	iteration	number	1351	MSE	0.1081	MAE	0.2159	Time	1105	72099
Sample		2048	iteration	number	1361	MSE	0.1031	MAE	0.2101	Time	1096	. 65966
Sample		2048	iteration	number	1371	MSE	0.1047	MAE	0.2126	Time	1099	.33114
Sample		2048	iteration	number	1381	MSE	0.1095	MAE	0.2185	Time	1104	. 92062
Sample	size	2048	iteration	number	1391	MSE	0.1035	MAE	0.2115	Time	1103	. 19352
Sample	size	2048	iteration	number	1401	MSE	0.1021	MAE	0.2140	Time	1097	. 98836
Sample		2048	iteration	number	1411	MSE	0.1021	MAE	0.2087	Time	1099	. 60818
Sample		2048	iteration	number	1421	MSE	0.1084	MAE	0.2187	Time	1100	. 57401
Sample	size	2048	iteration	number	1431	MSE	0.1028	MAE	0.2118	Time	1107	. 88703
Sample	size	2048	iteration	number	1441	MSE	0.1183	MAE	0.2276	Time	1097	.81885
Sample		2048	iteration	number	1451	MSE	0.1167	MAE	0.2214	Time	1092	. 97561
Sample		2048	iteration	number	1461	MSE	0.1000	MAE	0.2132	Time	1087	.07451
Sample	size	2048	iteration	number	1471	MSE	0.0984	MAE	0.2033	Time	1087	.09168
Sample	size	2048	iteration	number	1481	MSE	0.1054	MAE	0.2151	Time	1089	.06626
Sample	size	2048	iteration	number	1491	MSE	0.1091	MAE	0.2231	Time	1097	. 97787
Sample	size	2048	iteration	number	1501	MSE	0.1087	MAE	0.2163	Time	1109	.46273
Sample	size	2048	iteration	number	1511	MSE	0.1031	MAE	0.2139	Time	1085	. 12425
Sample	size	2048	iteration	number	1521	MSE	0.1202	MAE	0.2219	Time	1088	. 58561
Sample	size	2048	iteration	number	1531	MSE	0.1071	MAE	0.2114	Time	1099	. 15828
Sample	size	2048	iteration	number	1541	MSE	0.1010	MAE	0.2106	Time	1085	. 38723
Sample	size	2048	iteration	number	1551	MSE	0.1022	MAE	0.2112	Time	1087	. 52965
Sample	size	2048	iteration	number	1561	MSE	0.1099	MAE	0.2122	Time	1086	.60244
Sample	size	2048	iteration	number	1571	MSE	0.1115	MAE	0.2206	Time	1083	. 68754
Sample	size	2048	iteration	number	1581	MSE	0.1065	MAE	0.2205	Time	1083	. 16803
Sample	size	2048	iteration	number	1591	MSE	0.1024	MAE	0.2106	Time	1084	. 13910
Sample	size	2048	iteration	number	1601	MSE	0.1084	MAE	0.2176	Time	1082	. 43274
Sample	size	2048	iteration	number	1611	MSE	0.1139	MAE	0.2220	Time	1087	. 35585
Sample	size	2048	iteration	number	1621	MSE	0.0996	MAE	0.2153	Time	1083	.34660
Sample	size	2048	iteration	number	1631	MSE	0.1041	MAE	0.2144	Time	1081	.12120
Sample	size	2048	iteration	number	1641	MSE	0.1116	MAE	0.2132	Time	1083	. 45580
Sample	size	2048	iteration	number	1651	MSE	0.0942	MAE	0.2028	Time	1087	. 57948

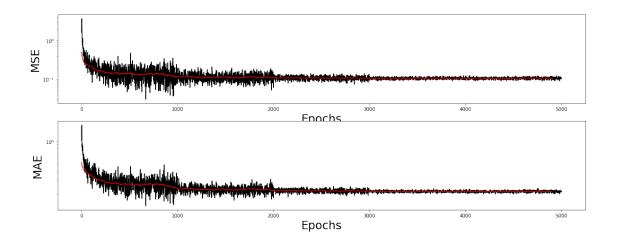
Sample	size	2048	iteration	number	1661	MSE	0.0965	MAE	0.2087	Time	1084.06949
Sample	size	2048	iteration	number	1671	MSE	0.1182	MAE	0.2265	Time	1096.07029
Sample	size	2048	iteration	number	1681	MSE	0.1047	MAE	0.2118	Time	1080.11555
Sample	size	2048	iteration	number	1691	MSE	0.1112	MAE	0.2187	Time	1084.47146
Sample	size	2048	iteration	number	1701	MSE	0.1085	MAE	0.2175	Time	1080.40070
Sample	size	2048	iteration	number	1711	MSE	0.1029	MAE	0.2116	Time	1089.06793
Sample	size	2048	iteration	number	1721	MSE	0.1048	MAE	0.2143	Time	1086.58671
Sample	size	2048	iteration	number	1731	MSE	0.1043	MAE	0.2177	Time	1085.12020
Sample	size	2048	iteration	number	1741	MSE	0.0996	MAE	0.2139	Time	1088.24205
Sample	size	2048	iteration	number	1751	MSE	0.1202	MAE	0.2346	Time	1083.65964
Sample	size	2048	iteration	number	1761	MSE	0.1038	MAE	0.2126	Time	1083.10604
Sample	size	2048	iteration	number	1771	MSE	0.1029	MAE	0.2137	Time	1084.07163
Sample	size	2048	iteration	number	1781	MSE	0.1051	MAE	0.2119	Time	1089.08486
Sample	size	2048	iteration	number	1791	MSE	0.1068	MAE	0.2185	Time	1088.00792
Sample	size	2048	iteration	number	1801	MSE	0.1065	MAE	0.2140	Time	1083.10675
Sample	size	2048	iteration	number	1811	MSE	0.1011	MAE	0.2090	Time	1086.73596
Sample	size	2048	iteration	number	1821	MSE	0.1098	MAE	0.2212	Time	1086.21597
Sample	size	2048	iteration	number	1831	MSE	0.1034	MAE	0.2134	Time	1084.23018
Sample	size	2048	iteration	number	1841	MSE	0.1055	MAE	0.2186	Time	1083.29868
Sample	size	2048	iteration	number	1851	MSE	0.1003	MAE	0.2076	Time	1088.36484
Sample	size	2048	iteration	number	1861	MSE	0.1006	MAE	0.2111	Time	1084.34581
Sample	size	2048	iteration	number	1871	MSE	0.0979	MAE	0.2096	Time	1089.08653
Sample	size	2048	iteration	number	1881	MSE	0.1018	MAE	0.2123		1086.16995
Sample	size	2048	iteration		1891	MSE	0.1030	MAE	0.2143		1084.01083
Sample	size	2048	iteration	number	1901	MSE	0.1185	MAE	0.2223	Time	1085.83569
Sample	size	2048	iteration	number	1911	MSE	0.1076	MAE	0.2150	Time	1093.05834
Sample	size	2048	iteration	number	1921	MSE	0.0982	MAE	0.2117	Time	1084.59115
Sample	size	2048	iteration	number	1931	MSE	0.1097	MAE	0.2175		1085.83283
Sample	size	2048	iteration	number	1941	MSE	0.1030	MAE	0.2135		1078.61328
Sample	size	2048	iteration		1951	MSE	0.1023	MAE	0.2072		1101.62401
Sample		2048	iteration		1961	MSE	0.0936	MAE	0.2043		1097.88537
Sample	size	2048	${\tt iteration}$		1971	MSE	0.1070	MAE	0.2166		1098.14763
Sample	size	2048	iteration	number	1981	MSE	0.1019	MAE	0.2133		1103.27553
Sample	size	2048	${\tt iteration}$	number	1991	MSE	0.1030	MAE	0.2122	Time	1098.01745
Sample	size	2048	iteration	number	2001	MSE	0.1049	MAE	0.2148	Time	1095.18837

1.6 6. PLOT LEARNING PERFORMANCE

The learning performance is plotted. The MSE, MAE, sample size, iteration number and iteration time are plotted against the number of timesteps.

Comment: 1. The parameter number_of_timesteps_for_average determines the length of the average. It must be a positive integer number.

```
In [8]: ### Plot learning performance
    number_of_timesteps_for_average = 100
    DeepCalib.plot_learning_performance(training_history, number_of_timesteps_for_average)
```



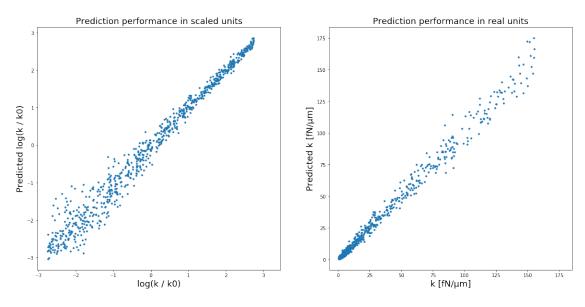
1.7 7. TEST DEEP LEARNING NETWORK ON NEW SIMULATED TRAJECTORIES

The deep learning network is tested on new simulated trajectories (parameters are defined in Section ??). The predicted values of the targets are plotted as function of their ground-truth values both in scaled and physical units.

Comments: 1. The parameter number_of_predictions_to_show determines the number of predictions that are shown.

In [9]: ### Test the predictions of the deep learning network on some generated trajectories
 number_of_predictions_to_show = 1000

%matplotlib inline
DeepCalib.plot_test_performance(simulate_trajectory, network, rescale_targets, number_of



1.8 9. SAVE DEEP LEARNING NETWORK

Comments: 1. The parameter save_file_name is the name of the file where the deep learnign network is saved. 2. By default, the network is saved in the same folder where DeepCalib is running.